NASA HPC Update

Supercomputers, Clusters & Hypercomputers
(Past, Present Future)

by

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Analytical & Computational Methods Branch
NASA Langley Research Center
Hampton Virginia

HPC Users Forum
Dearborn, Michigan
April 12-14 , 2004

Contents

Past HPC at NASA & Langley

Research: Langley, Ames, Glenn

Ops: JPL, Goddard, Dryden, Johnson, Kennedy, Marshall, MTC

Present Production (Cosmo + Center Clusters)

Research (CiCT + Center Clusters)

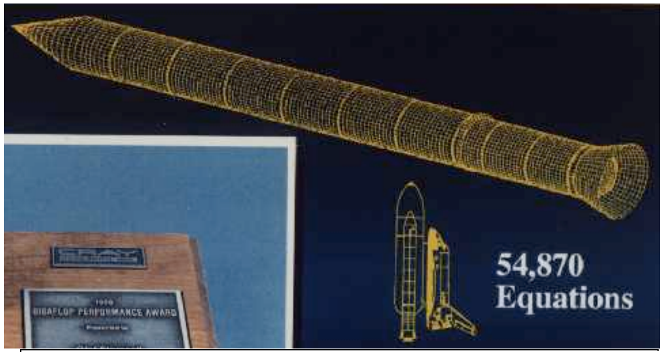
Future Clusters

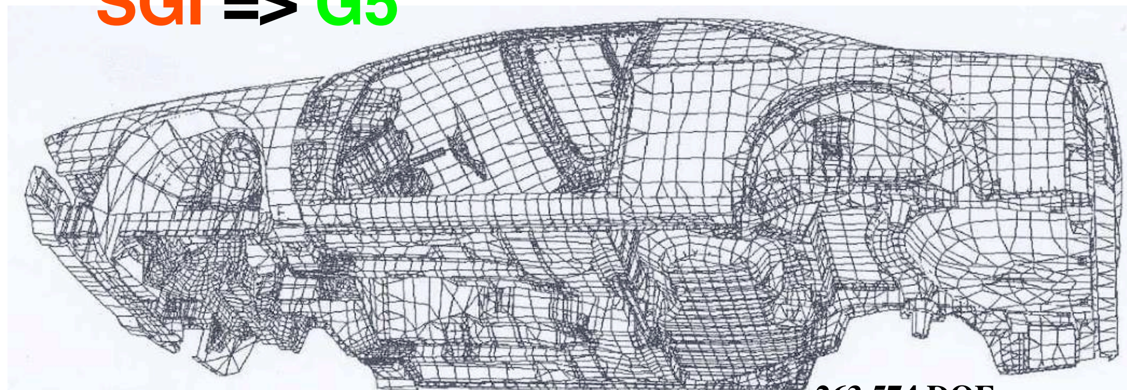
iNASA

Hypercomputers….

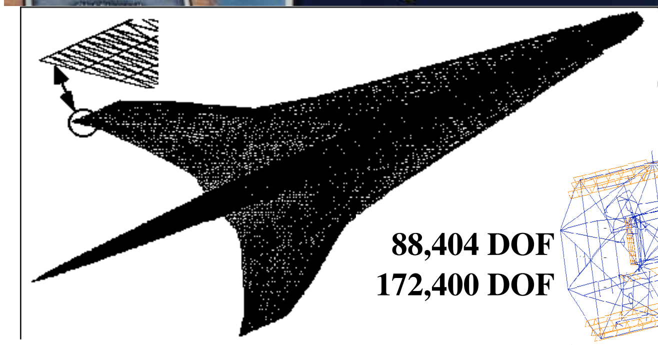
GPS Factor/Solve Time: [K]{u}={f}

SGI => G5

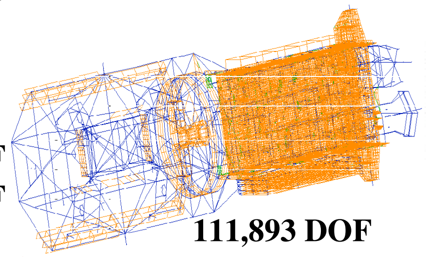




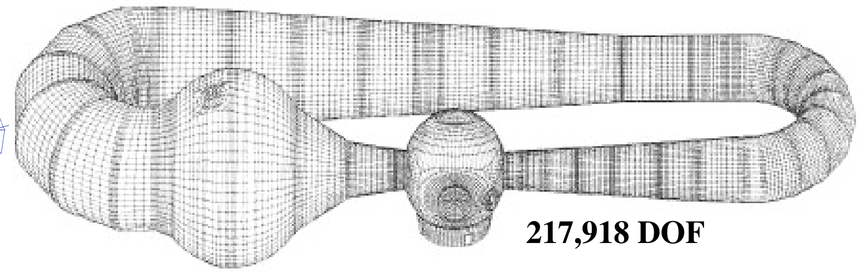
263,574 DOF



88,404 DOF
172,400 DOF



111,893 DOF

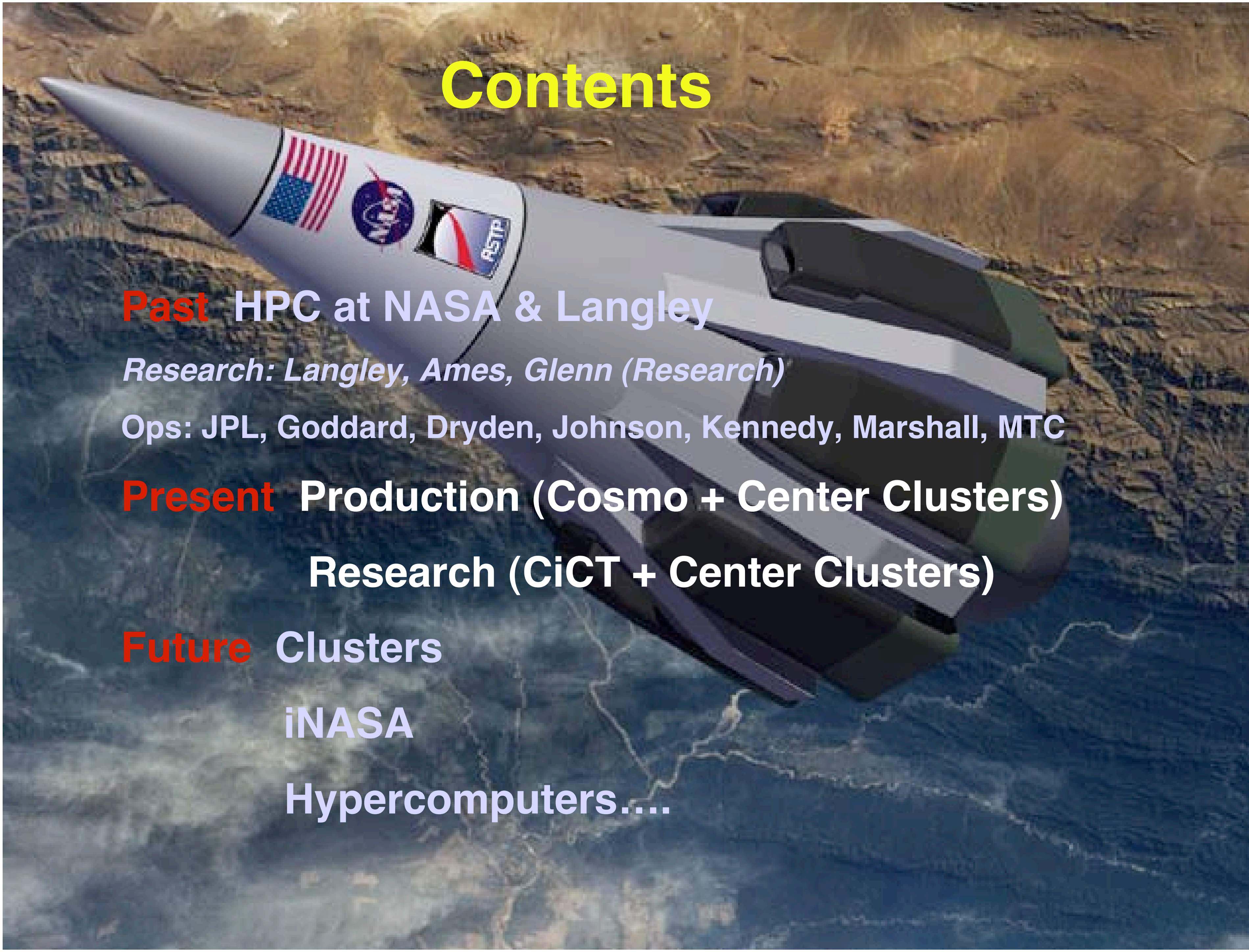


217,918 DOF

DOF/Eqns.	Terms ≠ 0	B-OPS	SGI/0.25G	G4/1GHz*	G5/2GHz	MF	Speedup
54,870	1.3 M	3.8	25.9 / 1.0	14.3 / 0.5	7.18 / 0.13	529	3.6 / 7.7
88,404	1.7 M	7.7	49.8 / 1.0	24.5 / 0.7	8.86 / 0.19	866	5.6 / 5.2
111,893	1.6 M	14.6	236.8 / 2.7	125.7 / 1.4	40.8 / 0.33	358	5.8 / 8.2
172,400	7.2 M	12.7	133.7 / 3.3	60.2 / 2.2	21.7 / 0.37	585	6.2 / 8.9
217,918	5.7 M	41.2	230.7 / 8.3	116.2 / 3.2	54.27/1.09	758	4.3 / 7.6
263,574	6.3 M	17.6	166.4 / 3.9	78.1 / 2.6	26.1/0.134	675	6.4 / 29

Error: $\|Ku-f\| < 10^{-10}$

*Laptop = Cray C90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iNASA
Hypercomputers….

A Revolution is Brewing in HPC

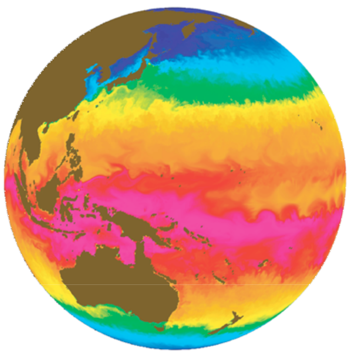
Accelerating Scientific Discovery and Understanding

The NASA Advanced Supercomputing (NAS) Division, working with NASA's Aeronautics and Earth Sciences Enterprises, has begun exploring new ways of doing high performance computing. The effort is focused on providing adequate HPC platforms with high availability to mission critical problems, in order to significantly accelerate the science discovery process in those areas.

Earth Sciences - The ECCO Project

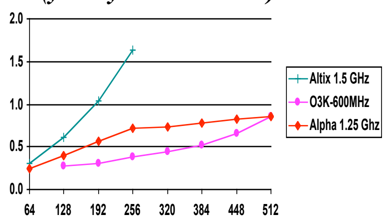
The Consortium for Estimating the Circulation and Climate of the Ocean (ECCO) is a joint venture between Jet Propulsion Laboratory, MIT, and the Scripps Institute of Oceanography. A major current effort is to execute a number of decadal ocean simulations using MIT's MITgcm code at 1/4 degree global resolution, or better. This effort is the first major project to use the new SGI Altix 512p single-system image (SSI) computer at NAS. NASA's new HPC system has provided a significant increase in throughput to the ECCO team. Some hint of this is seen in the performance chart (left). Additional optimizations are planned for this code on the Altix platform. These efforts are expected to increase performance to almost a simulated decade per day on 512 CPUs. This level of computing capability, dedicated to a core science team, can revolutionize the rate of scientific discovery, a process critical for national leadership in the sciences.

Cray X1 - 16p Supercomputer
The NAS team will be using this 192 GFLOP/s system to explore the performance envelop of "new age" vector supercomputers on a variety of NASA codes.



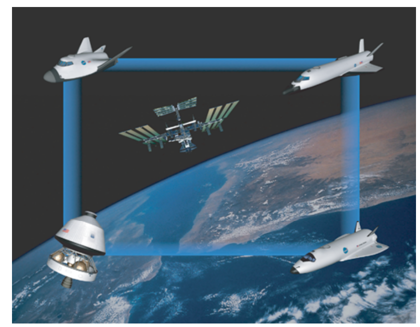
SGI Altix - 512p SSI System
The SGI Altix SSI system has been operational since 10/30/03. It is routinely scaling production applications to 512 CPUs with excellent results.

MITgcm Performance - 1/4 Degree
(yrs/day vs CPU Count)

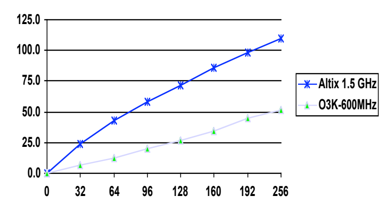


Aerosciences - The OSP and RTF Projects

A second major NAS effort to accelerate the time to solution for key mission programs, centers around work in the Aerosciences. NASA, in particular, needs extensive computational resources to address the specific needs of its Return to Flight (RTF) and Orbital Space Plane (OSP) projects. The NAS Division is working with NASA Enterprise leadership to define a small series of focused efforts in support of these activities. In the past, the OVERFLOW code has been essential for NASA and Aero industry needs in flow simulations over existing and notional designs. The Altix system has significantly improved the time to solution for this code. The chart (right) shows a comparison with previous best efforts.



OVERFLOW - 35M Point Problem
(GFLOP/s vs CPU Count)

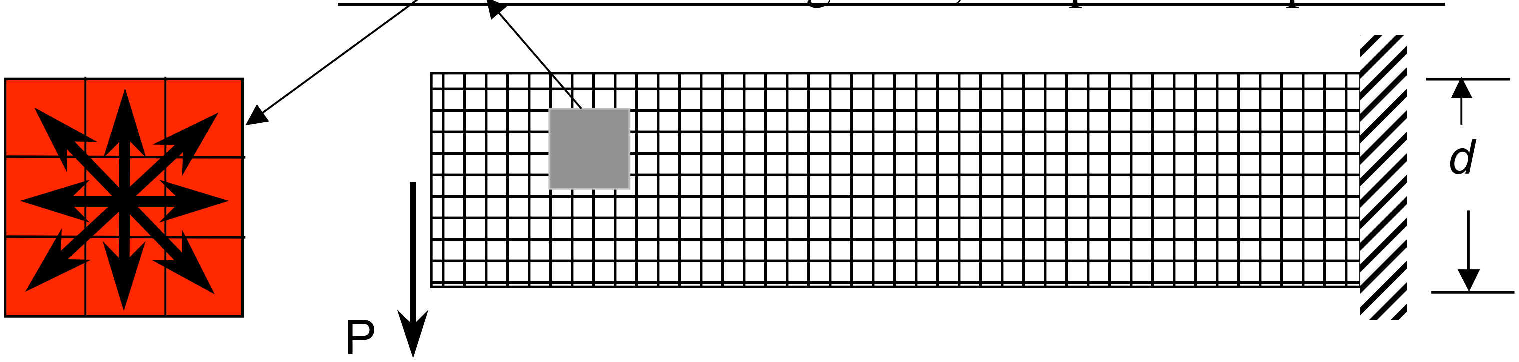


+ VT (Xserve) & Hypercomputers

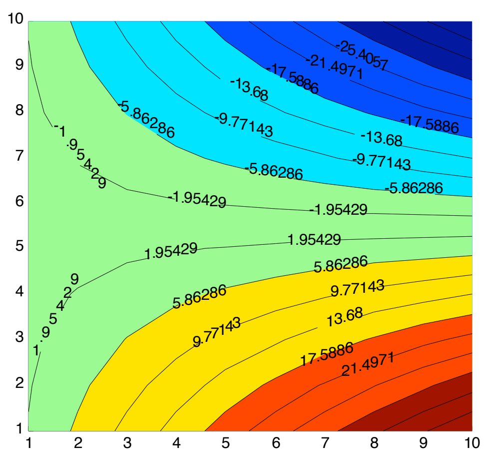
New Solution Methods

- Cellular Automata: Stephen Wolfram - *A New Kind of Science*
- Complexity via simple interactions **w/o PDEs**
- CFD => Structures

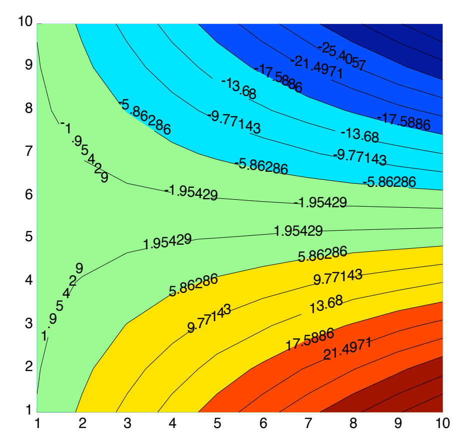
- Cell interacts with neighbors; one processor per cell



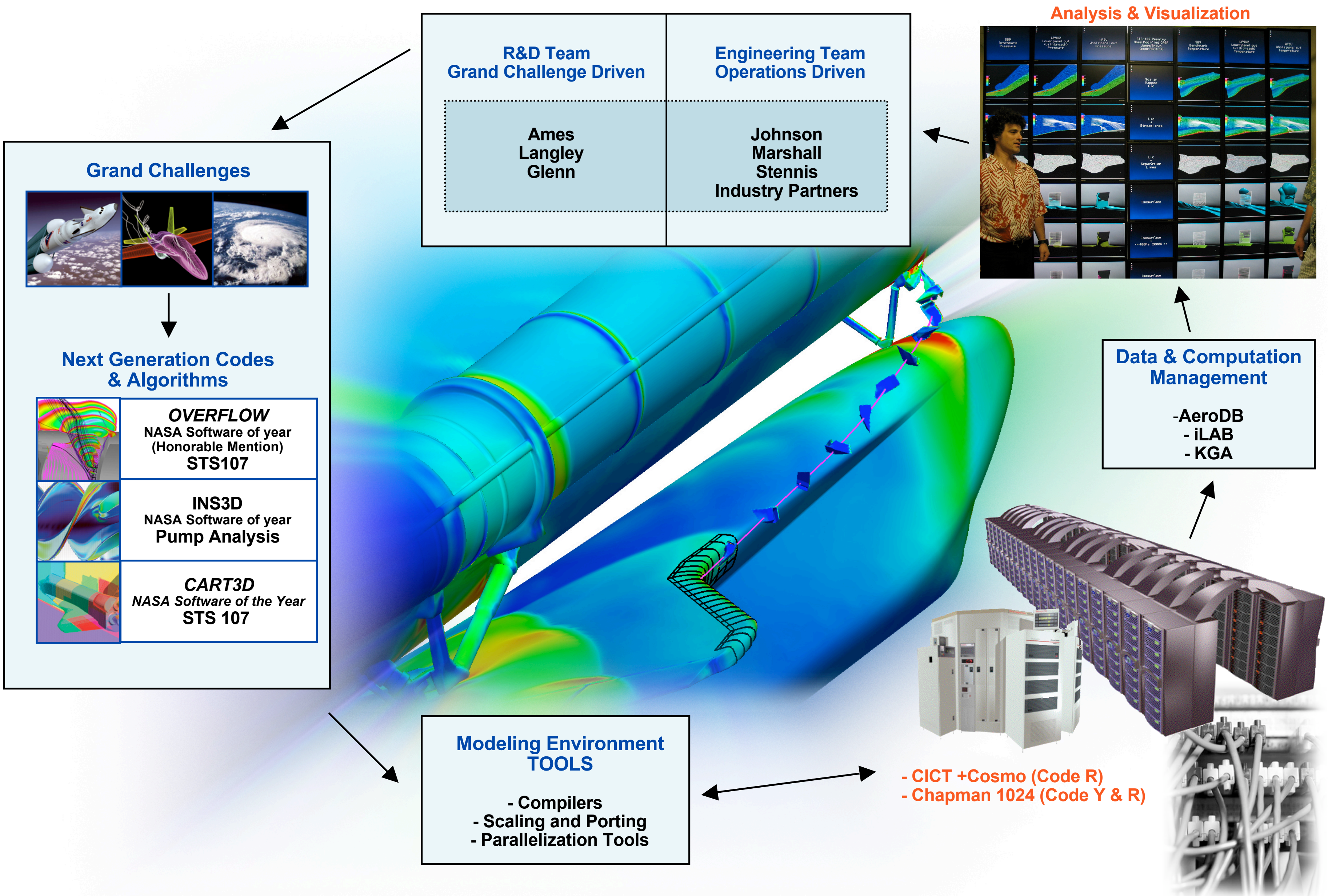
FEA solution



Cellular Automata solution



STS-107 Investigation Support



NASA-wide HPC Systems

SGI Altix: 128 Processors
(IA64 - 6 GFLOP/CPU)

Cray X1 : 64 Processors
(Custom - 12 GFLOP/CPU)

+ 128 processor Opteron System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ASTP

Langley Cluster Growth

Estimate by Joseph.H.Morrison@nasa.gov
Chair of Langley Cluster SIG

1200 - 1500 nodes on 2/04
440 nodes added since 6/03
50% increase in nodes/year

for several years

Other NASA Centers: Similar growth?

Why? 3x – 20x less to compute locally
Cost/CPU hour roughly 1/10

Chair, Langley Cluster SIG

Growing HPC Interest at Langley

LANGLEY Colloquium SERIES Since 1971

System X: Building the Virginia Tech Supercomputer

by Prof. Srinidhi Varadarajan

February 3, 2004, 2:00 P.M. in the H.J.E. Reid Auditorium.

TOP500® SUPERCOMPUTER SITES

Rank	Site Country/Year	Computer / Processors Manufacturer	R_{max} R_{peak}
1	Earth Simulator Center Japan/2002	**Earth-Simulator** / 5120 NEC	35860 40960
2	Los Alamos National Laboratory United States/2002	**ASCI Q - AlphaServer SC45, 1.25 GHz** / 8192 HP	13880 20480
3	Virginia Tech United States/2003	*X* **1100 Dual 2.0 GHz Apple G5/Mellanox Infiniband 4X/Cisco GigE** / 2200 Self-made	10280 17600

Many NASA G5 Xserve orders
Port of CFD & FE codes

The Sigma Series

A Forum on Science & Technology

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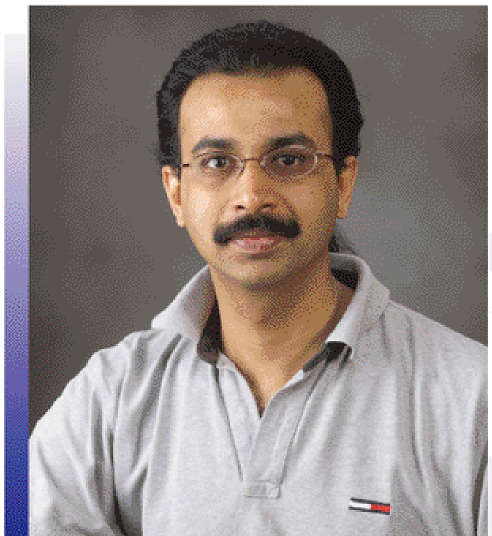


System X:
Building the Virginia Tech Supercomputer

Dr. Srinidhi Varadarajan

February 3, 2004
7:30 p.m.

Virginia Air and Space Center

System X was conceived in March, designed in July and, by October 2003, it achieved a sustained performance of 10.28 Teraflops, thus becoming the World's third-fastest supercomputer. System X has several novel features. It is the first scientific supercomputer with Apple technology, using 1100 Apple G5 platforms which employ the new IBM PowerPC 970 64-bit CPU. Secondly, System X uses a high-performance switched communications fabric called Infiniband. Finally, it is cooled by a hybrid liquid-air cooling system. System X was assembled in only three weeks for a very affordable price when compared to other world-class supercomputers. The speaker will present the motivation for System X, describe its architecture and discuss the challenges faced in building, deploying and maintaining a large-scale supercomputer.

Srinidhi Varadarajan received his Ph.D. in Computer Science from the State University of New York, Stony Brook in 2000. He is the Director of the Terascale Computing Facility at Virginia Tech and an Assistant Professor in the Department of Computer Science. Dr. Varadarajan is the architect of System X, the third fastest supercomputer in the world, located at the Terascale Computing Facility. Dr. Varadarajan's research is focused on transparent fault tolerance for massively parallel supercomputers, scaleable network emulation,

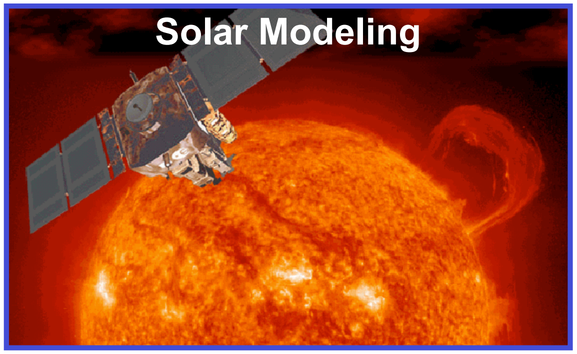
iNASA

(integrated NASA Architecture for Simulation and Analysis)

- **iNASA initiative will tackle NASA's *hardest Science and Engineering Modeling and Simulation Challenges* enabling unprecedented advances in multi-physics simulations with increased fidelity and resolution.**
  - **In concert with unique data created by science payloads, iNASA will create the capability to model and understand the processes that drive change in the Earth and in the Cosmos**
  - **Will allow, on a day-to-day basis, the capacity and capability to tackle simultaneously, at the limit of our engineering ability, problems that heretofore were untractable except on an episodic/emergency basis**

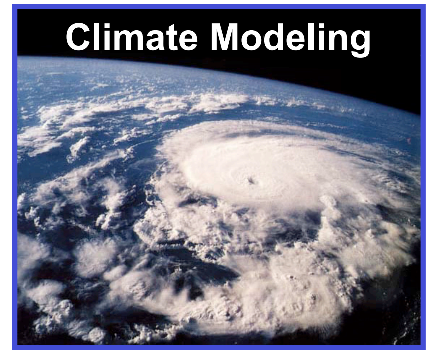
HPC Across NASA Enterprises

Space Science



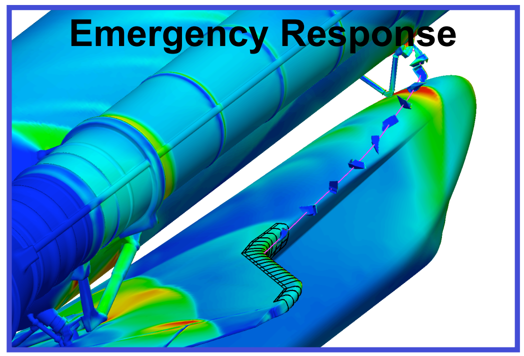
Exploration Systems

Earth Science

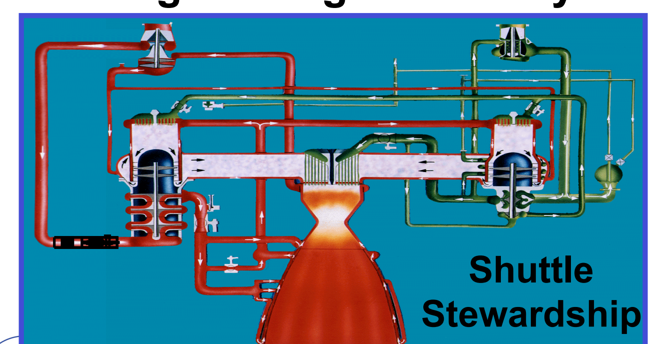


Biological and Physical Research

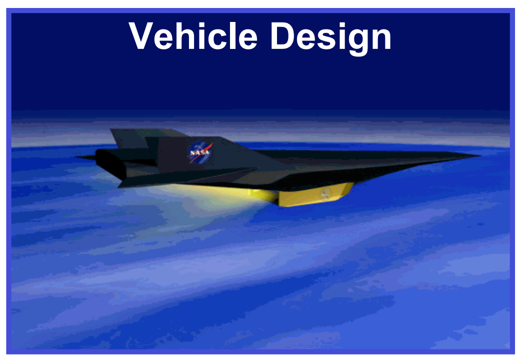
Space Flight



Engineering and Safety



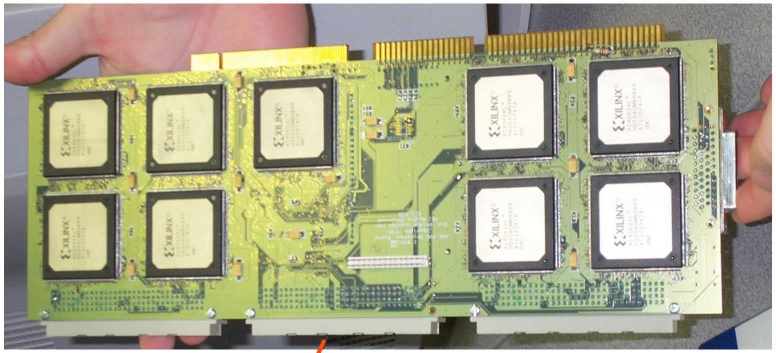
Aeronautics

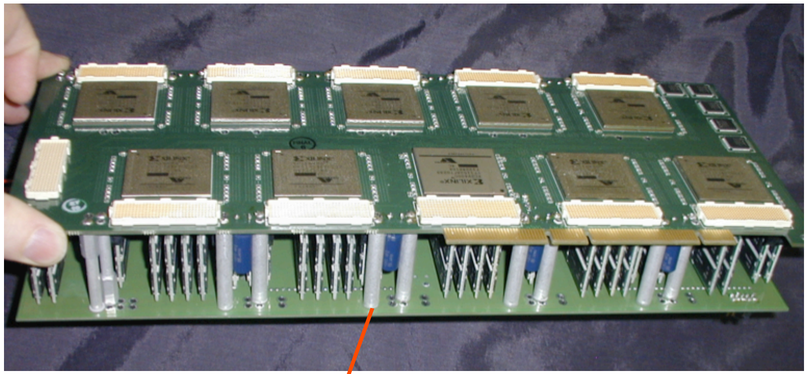


Each mission requires:

- Advanced models
- Model integration
- Efficient codes
- TF/PF Computation
- TB/PB data analysis, exploration, management
- Ensemble Analysis
- Science/engineering environments
- Remote resource access

Exploring Scientific Applications on Reconfigurable Hypercomputers





62K gates/FPGA

'02

Creativity & Innovation

'04

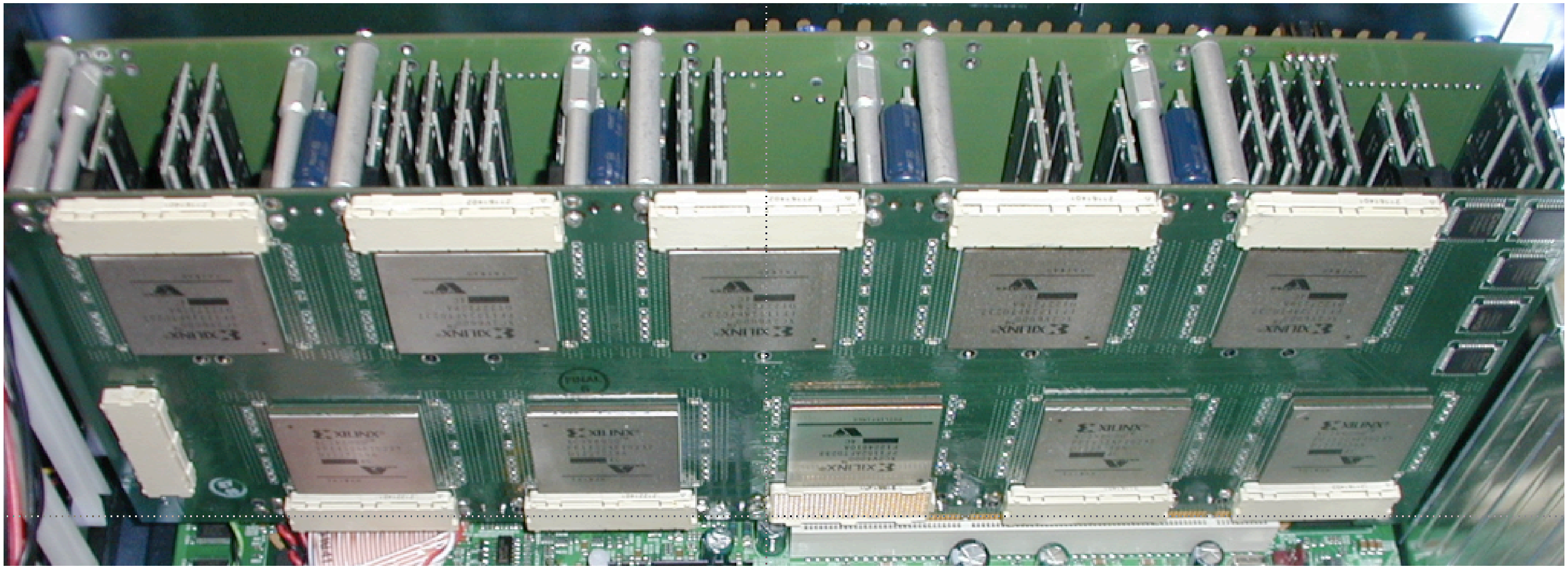
6M gates/FPGA
=> 60M soon

Computing Faster Without CPUs

GOAL: **Evaluate FPGA-based Hypercomputers for NASA Scientific Computations**

TEAM: **Drs. Olaf Storaasli & Jarek Sobieski**, **Principal Investigators**
Dr. Robert Singleterry, Dave Rutishauser, Joe Rehder, Garry Qualls
Shaun Foley-*MIT*, William Fithian-*Harvard*, Siddhartha Krishnamurthy-*VT*
Cris Kania-*VT*, Patrick Butler-*VT*, Hoy Loper-GS, Neha Dandawate-*UVA*,
Kristin Barr-*JPMorgan*, Robert Lewis-*Morehouse* , Vincent Vance-*VT* *+2 more*

PARTNERS: ***Starbridge Systems*, NSA, USAF, MSFC, *AlphaStar***



Langley-Starbridge Systems (SBS) Collaboration

- 1st SBS Hypercomputers @Langley (β-site: early H/W & S/W)
  ~ 1st Cray Supercomputer @LANL (8MB, 160MF, no O/S)

- **Langley**:
  - *application utilities & algorithms*
  - *identify bugs, recommend changes & utilities to SBS*
  - *coordinate with partners: NSA, USAF, MFSC, VPI*

  SC89 (GigaFLOP Award) Rollwagen "NASA saved Cray $2M"

- **Starbridge**:
  - *implement NASA suggestions*

==> **Make FPGAs better tool for NASA applications**

FPGA Computing

MetaLib

Traditional CPU

Sequential: 1 operation/cycle

Fixed gates & data types

Wasteful: 99% gates idle/cycle

yet all draw power

Software: Text

do i = 1, billion

c= a+b

end do

26 MFLOPS/250 MHz SGI

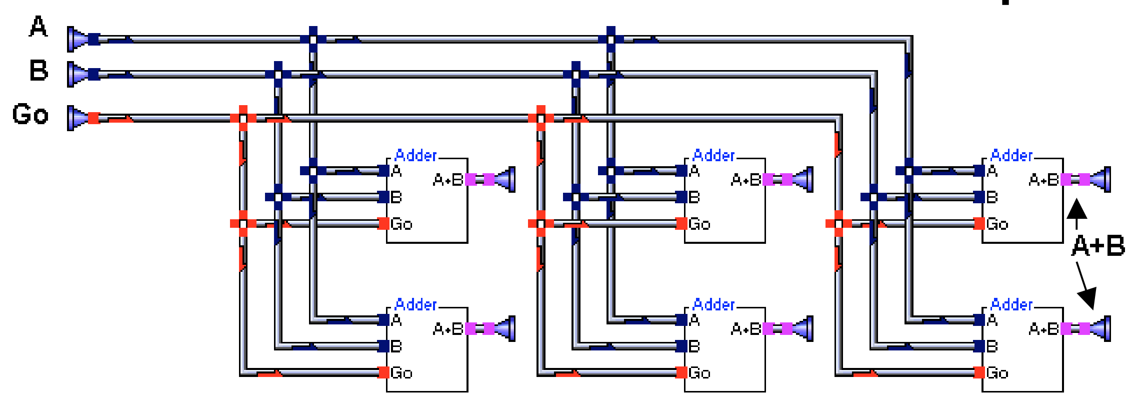
FPGA

Parallel: inherent

Dynamic gates & data types

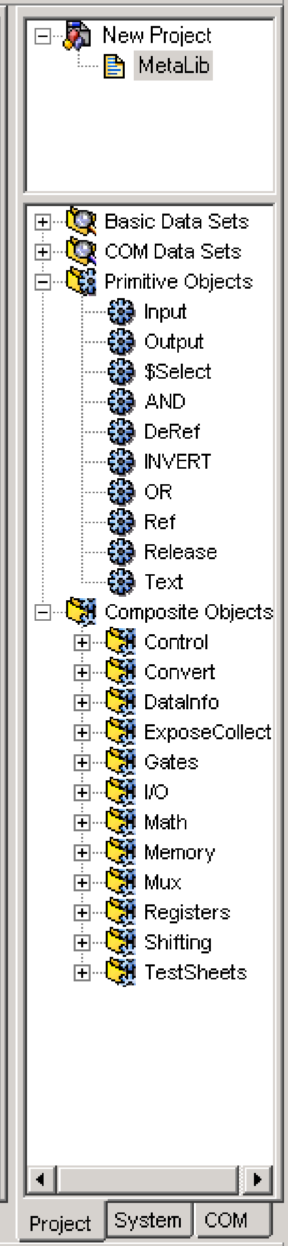
Efficient: Optimizes gates to task

Gateware: VIVA Icons & Transports



47+ GFLOPS/64 MHz FPGA

329+ GFLOPS/10 FPGA board



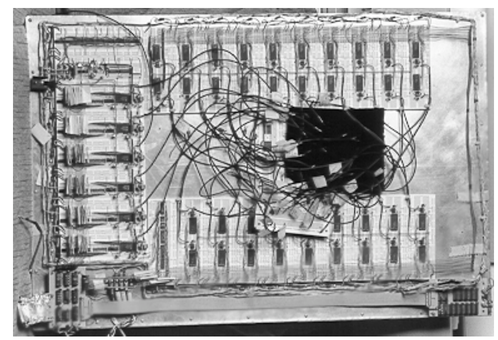
I2ADL Editor Data Set Editor

Start C:\Viva Viva 2.0 2:58 PM

Algorithms Developed*

- **Matrix Algebra**: {V}, [M], *$\{V\}^T\{V\}$, [M]x[M],GCD,…*
  - **n!** => Probability: Combinations/Permutations
  - **Cordic** => Transcendentals: sin, log, exp, cosh…
- ***$\partial y/\partial x$ & $\int f(x)dx$*** => Runge-Kutta: CFD, Newmark Beta: CSM
- **Matrix Equation Solvers**: $[A]\{x\} = \{b\}$ - Gauss & Jacobi
  - **Dynamic Analysis**: $[M]\{\ddot{u}\} + [C]\{\dot{u}\} + [K]\{u\} + NLT = \{P(t)\}$
- **Analog Computing**: digital accuracy
  - **Nonlinear Analysis**: Analog simulation

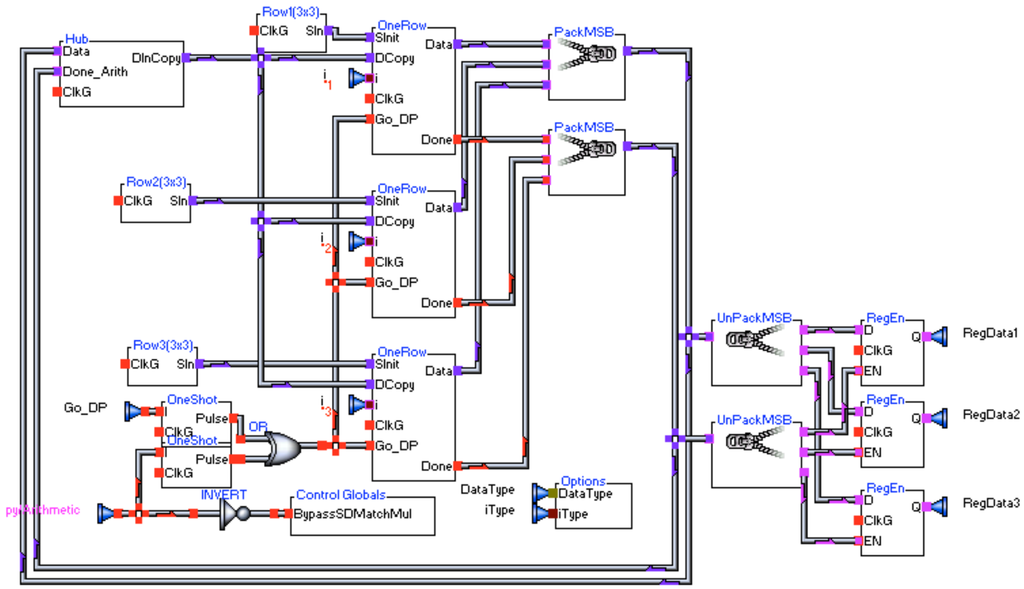
    avoids Non-Linear Term solution time



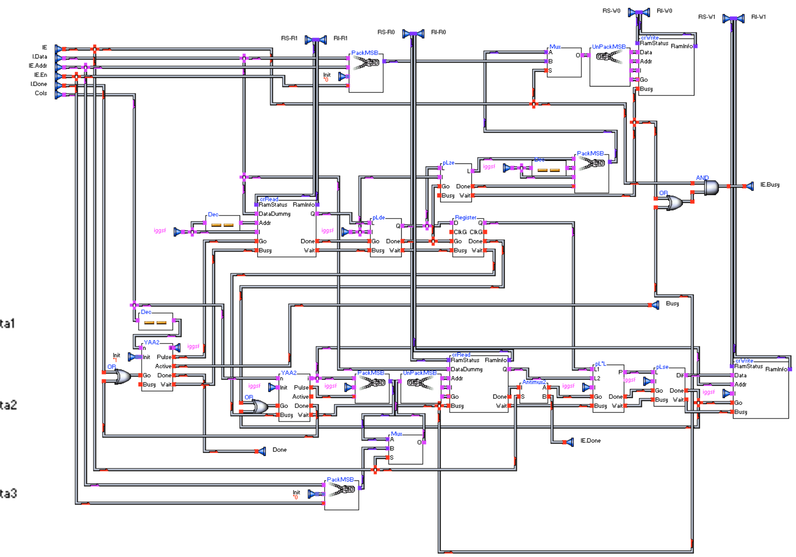
* Google: Publications Storaasli

Applications: VIVA Code

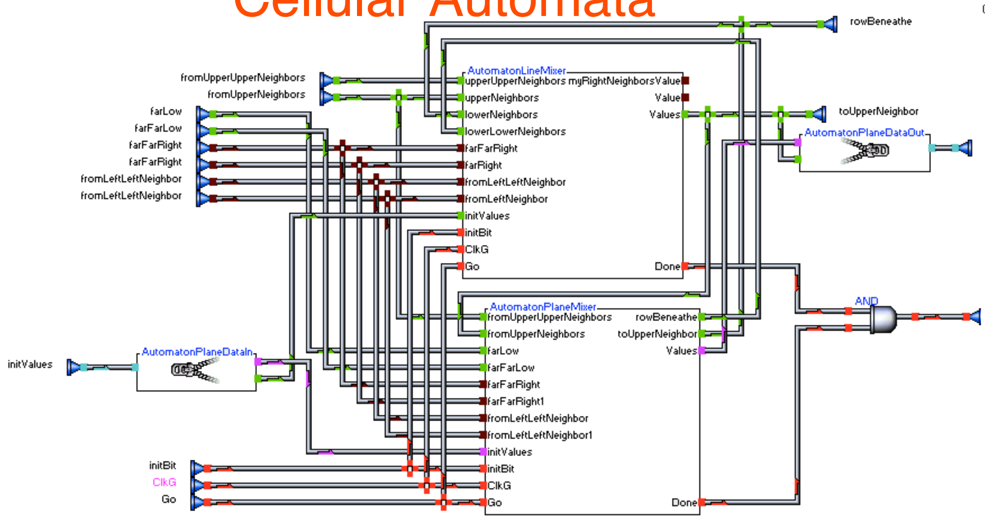
Jacobi Matrix Solver



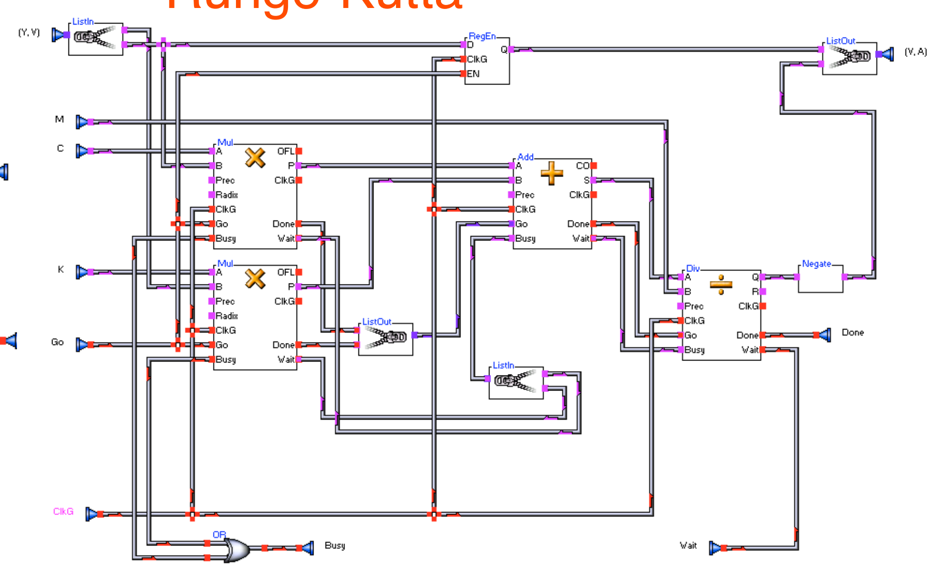
Gauss Matrix Solver



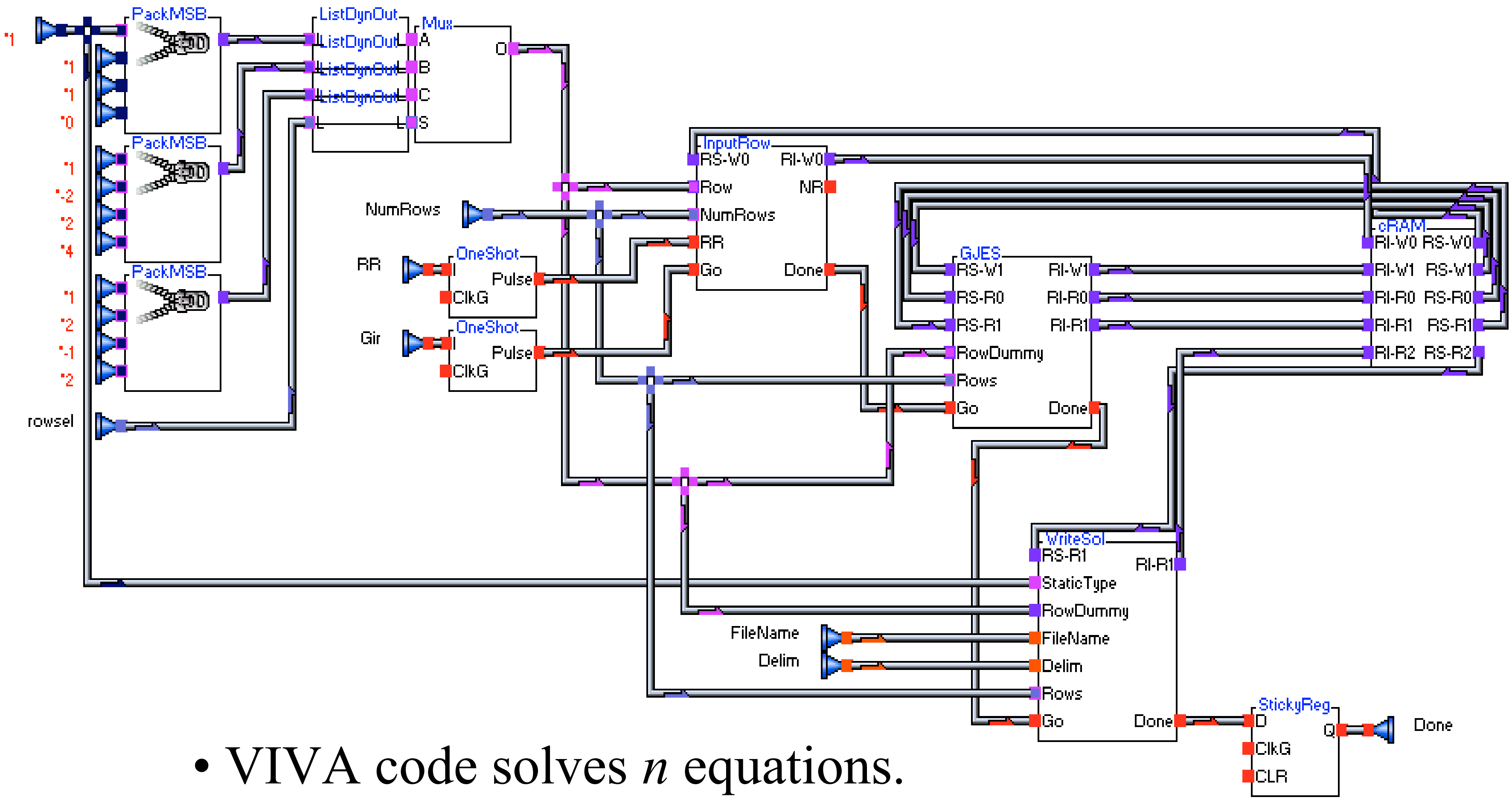
Cellular Automata



Runge-Kutta



Gauss-Jordan **A**x = **B** Solver



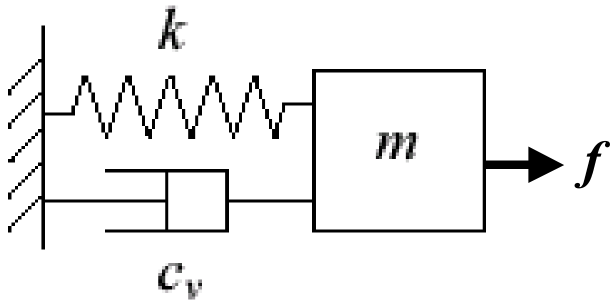
- VIVA code solves n equations.

Ex:

$$
\begin{aligned}
x_0 + x_1 + x_2 &= 0 \\
x_0 - 2x_1 + 2x_2 &= 4 \\
x_0 + 2x_1 - x_2 &= 2
\end{aligned}
\quad \Longrightarrow \quad
\begin{aligned}
x_0 &= 4 \\
x_1 &= -2 \\
x_2 &= -2
\end{aligned}
$$

- Run on hypercomputer emulator, then FPGA

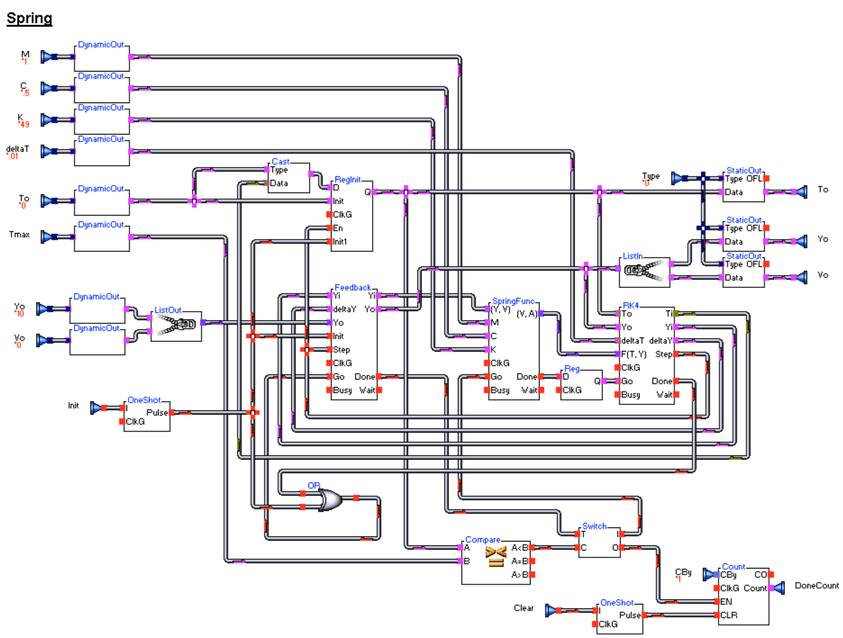
Spring-Mass Solver

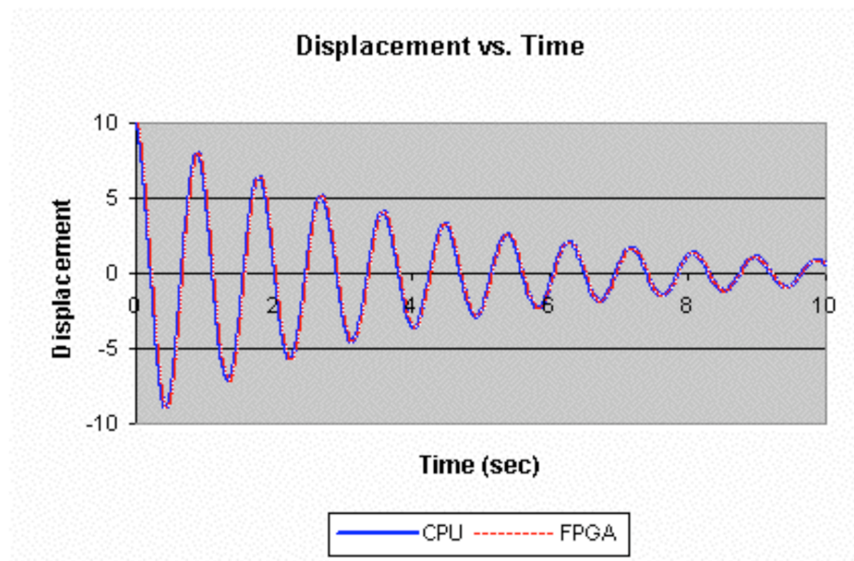


Method: 4-stage Runge-Kutta

$$\frac{du}{dt} = f(u,t) \qquad y(x_0) = y_0$$

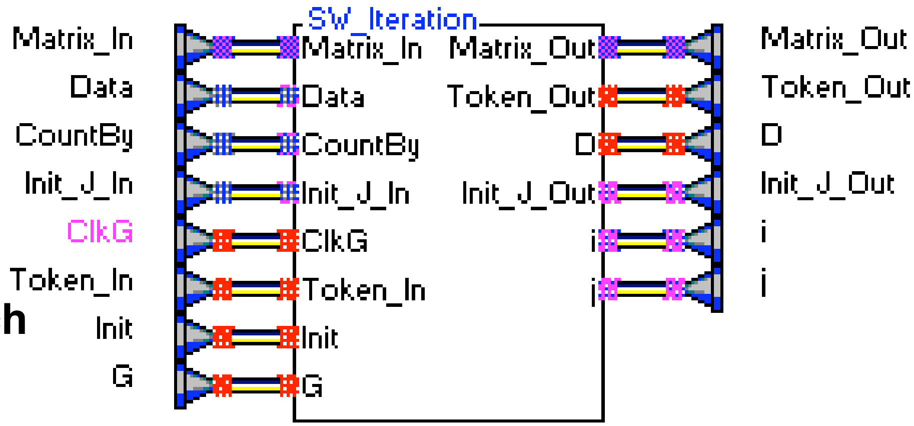
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_1)$$
$$k_3 = hf(x_n + \tfrac{1}{2}h, y_n + \tfrac{1}{2}k_2)$$
$$k_4 = hf(x_n + h, y_n + k_3)$$
$$x_{n+1} = x_n + h$$
$$y_{n+1} = y_n + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$



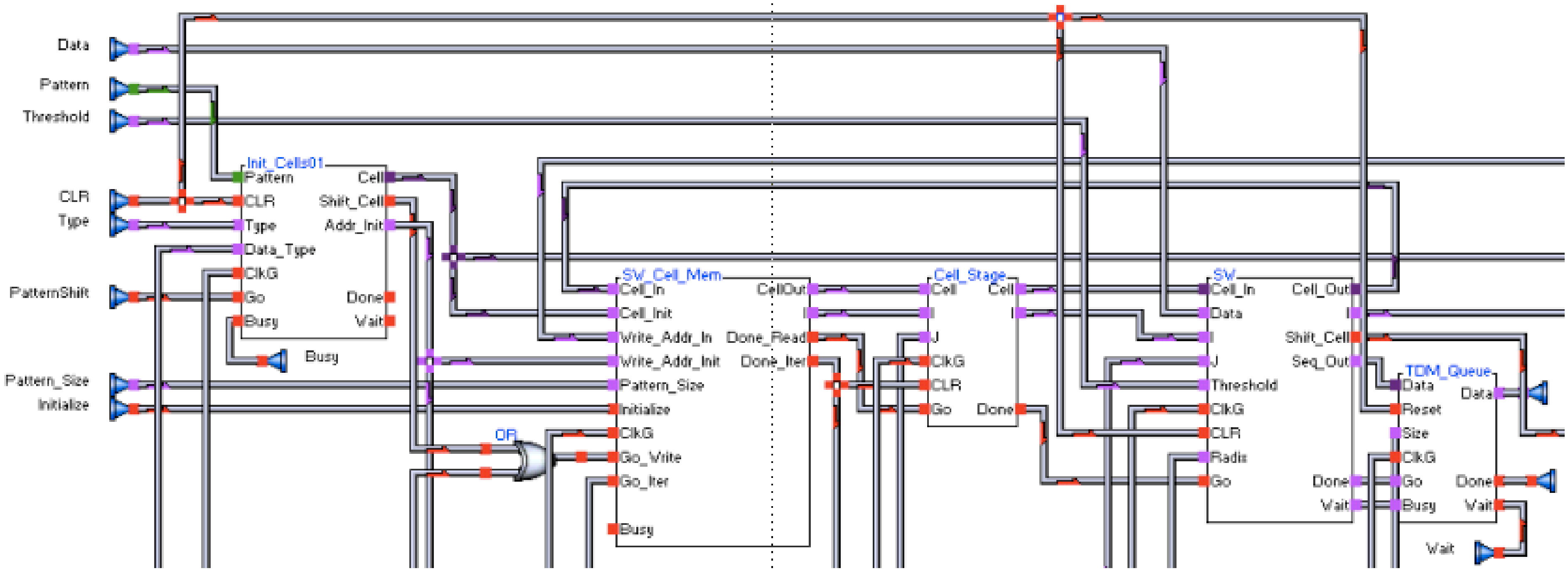


Smith Waterman Algorithm
(NCI Compares 2 DNA sequences)

stream of cells*
ref character
 # iterations, radix
iteration index
system clock
pulse before cells
pulse before search
for each cell
*** Keep full for efficiency**



newly-computed cell
for next iteration
new cell
for next interation
current row
current column



Olaf.O.Storaasli@nasa.gov

FPGA SW Performance

7 FPGAs, on HC62, compute SW cells in parallel

(each FPGA computes 64 iterations/cycle)

⇒ 448 parallel SW_Iterations @ 25 Mhz*

⇒ 25M * 448 = **11.2 billion SW steps/sec**

**conservative: may increase clock via VIVA*

VIVA adds on 1 FPGA

Adds-parallel	16	32	128	256	512	640
% FPGA used	1	2	8	16	41	51
Billion Ops	4	8	34	77	154	192

⇒1000 adds/clock cycle

(most CPUs limited to 1-3 ops/cycle)

Summary

NASA exploits HPC mix

✓ Production & Research Computing

✓ NASA-wide & Center Clusters

✓ Traditional & "far out" G5s & FPGAs

HPC future bright at NASA as capability/$ increases

More=> Google : **Publications Storaasli**